Experimental Math: Pure or Applied Mathematics?

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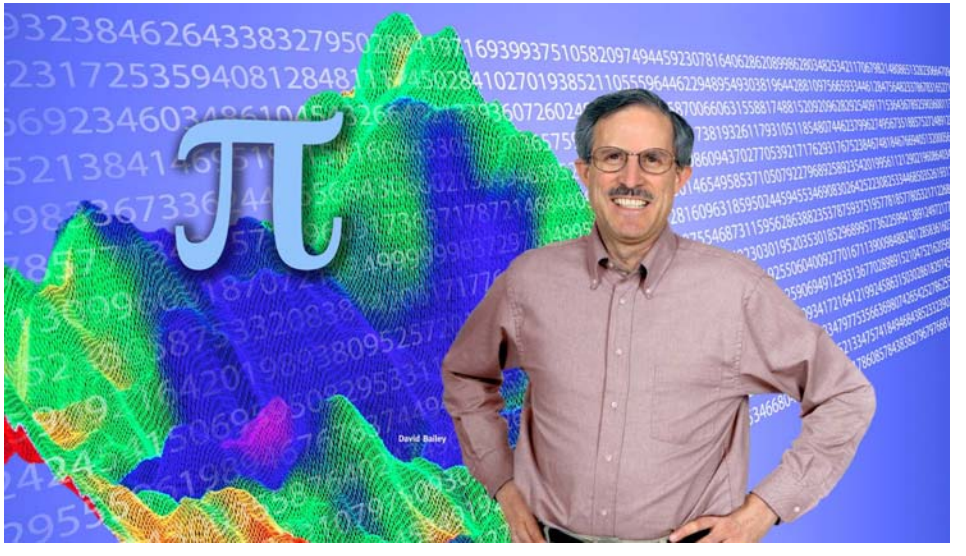


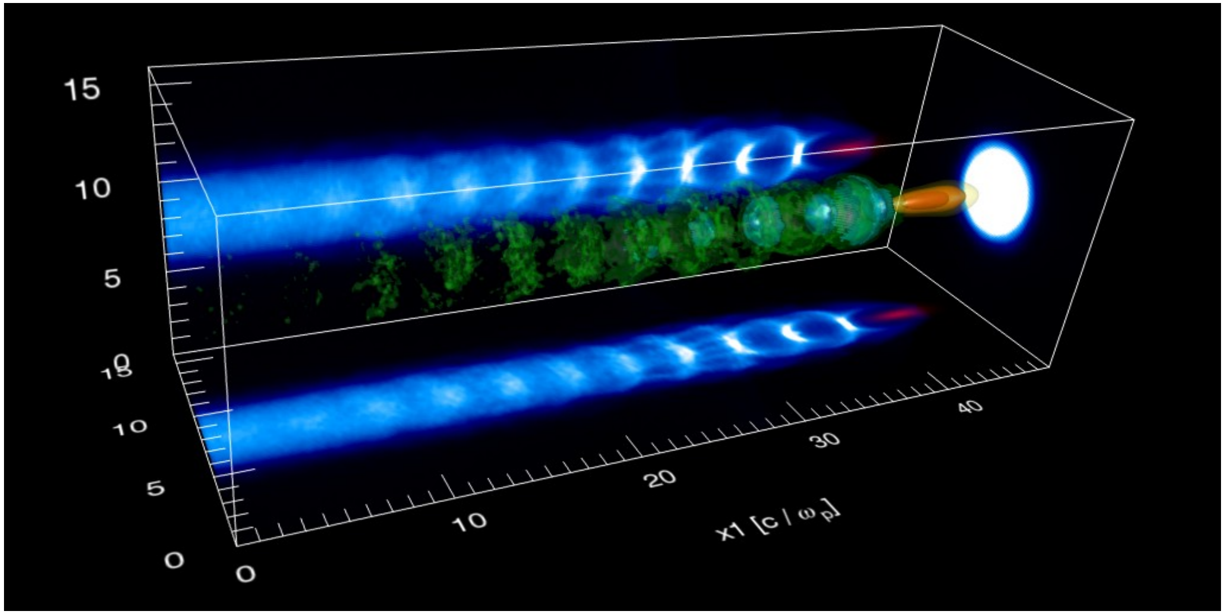
"All truths are easy to understand once they are discovered; the point is to discover them." – Galileo Galilei

The NERSC Computer Center at the Berkeley Laboratory

- Seaborg: 6656-CPU IBM P3 system, 10 Tflop/s peak, 7.8 Tbye memory.
- Bassi: 976-CPU IBM P5 system, 6.7 Tflop/s peak, 3.5 Tbyte memory.
- Jacquard: 640-CPU Opteron cluster, 2.8 Tflop/s peak, 1.9 Tbyte memory.
- A new, more powerful system is being procured; will be installed in 2006.

Applied Math Computations at NERSC: Accelerator Physics

- 3D simulations (such as ORIRIS shown below) have helped experimenters produce 100 MeV beams with significantly improved beam quality.
- Computations involve both dense and sparse linear algebra.
- Presently using 2 million CPU-hours annually.
- Future needs: at least 10 million CPU-hours annually.



Graphic: R. A. Fonseca (IST Portugal), F. S. Tsung (UCLA), and S. Deng (USC)

Climate Modeling

Characteristics:

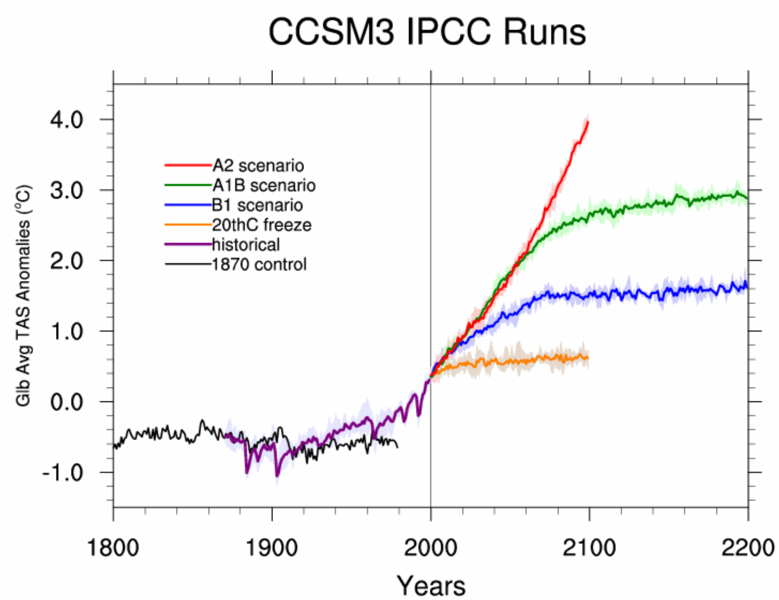
- Hydrodynamics, radiation transfer, thermodynamics, chemical reactions.
- Large finite difference methods, on regular spatial grids.
- Short- to medium-length FFTs are used, although these may be replaced in future.

Current state-of-the-art:

- Atmosphere: 1.4 horizontal deg spacing, with 26 vertical layers.
- Ocean: 1 degree spacing, 40 vert layers.
- Currently one simulated day requires 140 seconds on 208 CPUs.

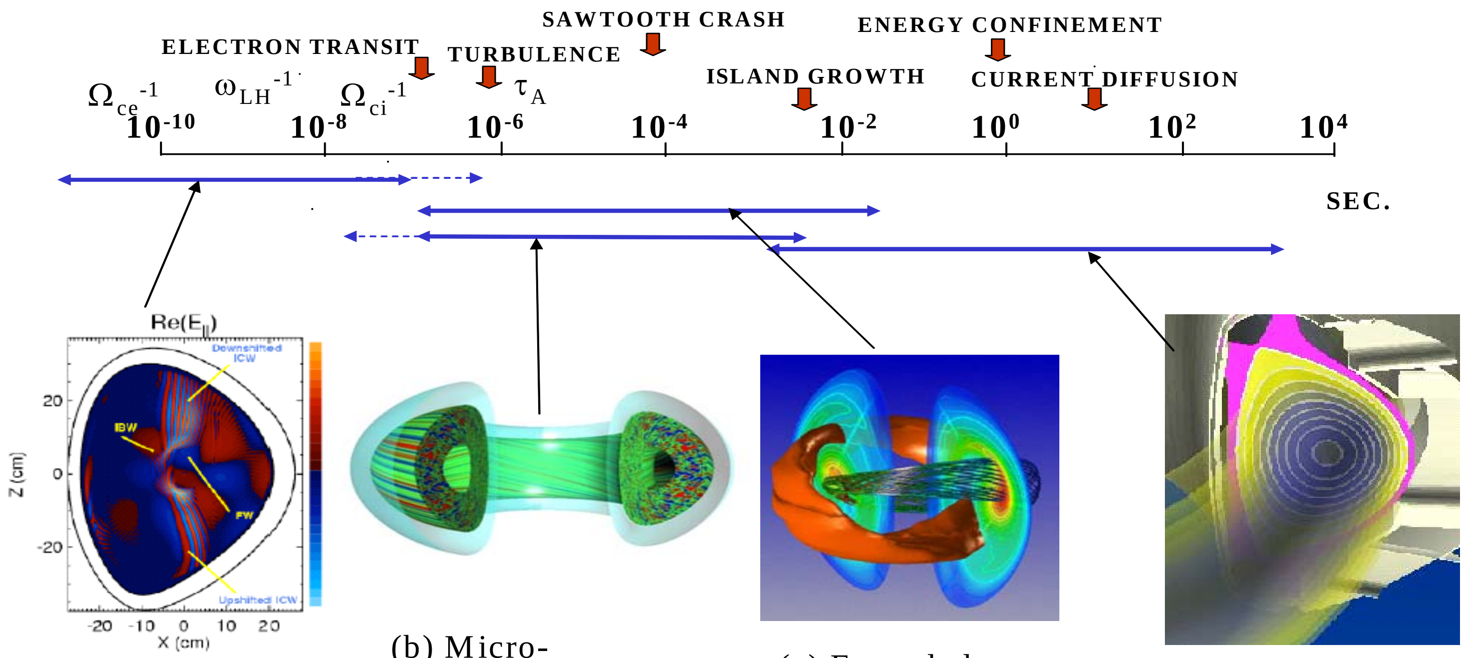
Future requirements:

- 800-1000X current requirements.



Graphic: G. Meehl, J. Arblaster, et al (NCAR)

Fusion Reactor Simulations



(a) RF codes

(b) Micro-turbulence codes

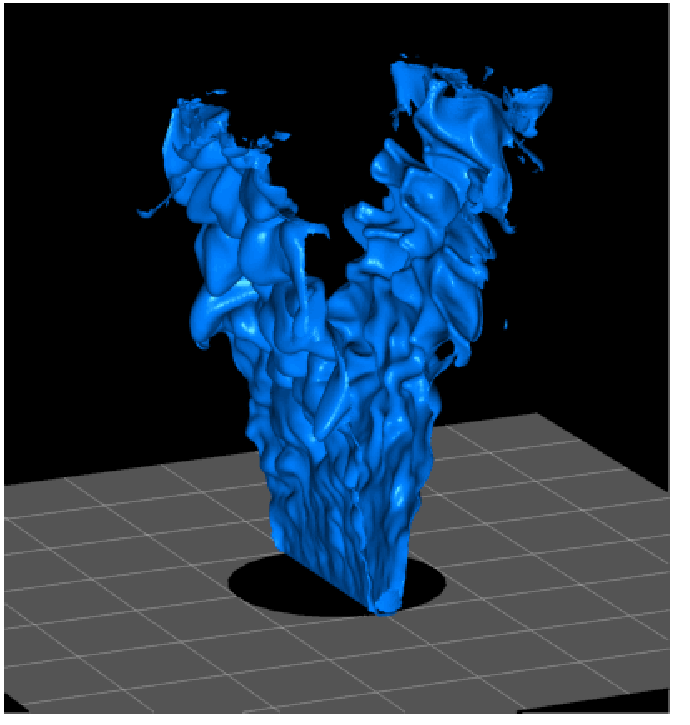
(c) Extended-MHD codes

(d) Transport Codes

- Regular and irregular access computations. Graphic: S. Jardin, et al (PPPL)
- Adaptive mesh refinement.
- Advanced nonlinear solvers for stiff PDEs.
- Current: 230 Gbyte memory, 1.3 hours on 1 Tflop/s system (larger problems require 8 hours).
- Future: 576 Tbyte memory, 160 hours on 1 Pflop/s system.

Combustion Simulation

- Span huge range in time and length scales (10^9), requiring large and adaptively-managed meshes.
- Explicit finite difference, finite volume and finite element schemes for systems of nonlinear PDEs.
- Implicit finite difference, finite volume and finite element schemes for elliptic and parabolic PDEs (iterative sparse linear solvers).
- Lagrangian particle methods.

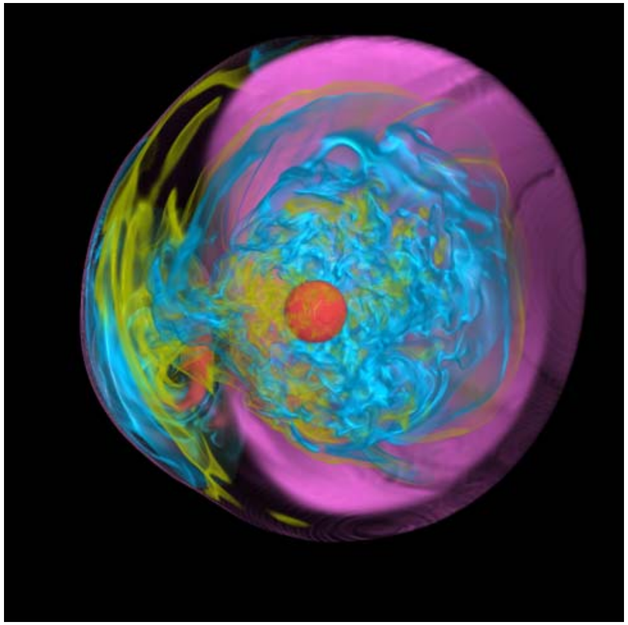


Graphic: J. Bell, M. Day, et al (LBNL)

Future requirements will strain the largest systems.

Astrophysics Simulation and Data Analysis

- Multi-physics and multi-scale phenomena.
- Large dynamic range in time and length.
- Requires adaptive mesh refinement.
- Dense linear algebra.
- FFTs and spherical harmonic transforms.



Supernova simulation:

- Future 3-D model calculations will require 1,000,000 CPU-hours per run, on 100 Tflop/s peak system.

Analysis of cosmic microwave background data:

- WMAP (now) — 3×10^{21} flops, 16 Tbyte mem
- PLANCK (2007) — 2×10^{24} flops, 1.6 Pbyte mem
- CMBpol (2015) — 1×10^{27} flops, 1 Ebyte mem

Graphic: T. Mezzacappa, J. Blondin, K.-L. Ma, et al (ORNL)

Common Characteristics of Modern Computational/Applied Math

- The ultimate objective is to advance the applied discipline:
  - Physics, chemistry, astronomy, biology, climate, engineering, biotech.
- Advanced numerical algorithms and computational techniques:
  - FFTs, dense linear algebra, sparse linear algebra, iterative solvers, multigrid, highly parallel processing, dynamic data structures, etc.
- State-of-the-art calculations require highly parallel computers:
  - Enormous computational requirements are common.
  - 1000+ CPUs are used in many calculations.
- A pragmatic attitude prevails: “If it works, use it.”
  - Some combinatorial optimization algorithms are observed to work significantly better in practice than theory might suggest.
  - Gaussian elimination with partial pivoting is not guaranteed to work in all cases, yet works fine in real applications.
  - The QR algorithm was used for many years before it was found to cycle in a simple 4x4 case. A proof of convergence is still elusive.

Experimental Math as Pure Mathematics

- New formula for pi.
- Other BBP-type formulas.
- Recent proof of non-existence of non-binary BBP formulas for pi.
- Euler sums and multivariate zeta sums.
- Apery-type identities.
- Ramanujan-like identities.
- Definite integrals.
- Connection between BBP formulas and normality.

In his March 2006 *Scientific American* article on the limits of mathematics, Gregory Chaitin cites *Mathematics by Experiment* among his five references.

The PSLQ Integer Relation Algorithm

Let (x_n) be a vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$$

At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm.

PSLQ was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

High-precision arithmetic software is required: at least d x n digits, where d is the size (in digits) of the largest of the integers a_k.

Authors: Helaman Ferguson, Stephen Arno and DHB

The BBP Formula for Pi

In 1996, a computer program running the PSLQ algorithm discovered this formula for pi:

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

This formula permits one to directly calculate binary or hexadecimal (base-16) digits of pi beginning at an arbitrary starting position n, without needing to calculate any of the first n-1 digits.

This formula is now used in the G95 compiler.

Authors: Peter Borwein, Simon Plouffe and DHB

Some Other Similar BBP-Type Identities

$$\pi^2 = \frac{1}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{144}{(6k+1)^2}-\frac{216}{(6k+2)^2}-\frac{72}{(6k+3)^2}-\frac{54}{(6k+4)^2}+\frac{9}{(6k+5)^2}\right)$$

$$\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}\left(\frac{243}{(12k+1)^2}-\frac{405}{(12k+2)^2}-\frac{81}{(12k+4)^2}-\frac{27}{(12k+5)^2}\right.$$
$$\left.-\frac{72}{(12k+6)^2}-\frac{9}{(12k+7)^2}-\frac{9}{(12k+8)^2}-\frac{5}{(12k+10)^2}+\frac{1}{(12k+11)^2}\right)$$

$$\zeta(3) = \frac{1}{1792}\sum_{k=0}^{\infty}\frac{1}{2^{12k}}\left(\frac{6144}{(24k+1)^3}-\frac{43008}{(24k+2)^3}+\frac{24576}{(24k+3)^3}+\frac{30720}{(24k+4)^3}\right.$$
$$-\frac{1536}{(24k+5)^3}+\frac{3072}{(24k+6)^3}+\frac{768}{(24k+7)^3}-\frac{3072}{(24k+9)^3}-\frac{2688}{(24k+10)^3}$$
$$-\frac{192}{(24k+11)^3}-\frac{1536}{(24k+12)^3}-\frac{96}{(24k+13)^3}-\frac{672}{(24k+14)^3}-\frac{384}{(24k+15)^3}$$
$$+\frac{24}{(24k+17)^3}+\frac{48}{(24k+18)^3}-\frac{12}{(24k+19)^3}+\frac{120}{(24k+20)^3}+\frac{48}{(24k+21)^3}$$
$$\left.-\frac{42}{(24k+22)^3}+\frac{3}{(24k+23)^3}\right)$$

$$\frac{25}{2}\log\left(\frac{781}{256}\left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}}\right)^{\sqrt{5}}\right) = \sum_{k=0}^{\infty}\frac{1}{5^{5k}}\left(\frac{5}{5k+2}+\frac{1}{5k+3}\right)$$

Authors: Peter Borwein, Simon Plouffe, David Broadhurst, Richard Crandall and DHB

Is There a Base-10 Formula for Pi?

Note that there is both a base-2 and a base-3 BBP-type formula for π^2. Base-2 and base-3 formulas are also known for a handful of other constants.

Question: Is there any base-n ($n \neq 2^b$) BBP-type formula for π?

Answer: No. This is ruled out in a 2004 paper.

This does not rule out some completely different scheme for finding individual non-binary digits of π.

Authors: Jon Borwein, David Borwein and Will Galway

Multivariate Zeta Sums

Consider this example:

$$S_{2,3} = \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + (-1)^{k+1}\frac{1}{k}\right)^2 (k+1)^{-3}$$

$$= \sum_{\substack{0<i,j<k \\ k>0}} \frac{(-1)^{i+j+1}}{ijk^3} = -2\,\zeta(3,-1,-1) + \zeta(3,2)$$

Using the EZFACE+ tool on the CECM website, one obtains the value:

```
0.1561669333811769158810359096879881936857767098403038729
  57529354497075037440295791455205653709358147578...
```

Using PSLQ, one can then find this evaluation:

$$S_{2,3} = 4\,\mathrm{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30}\log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4\log(2) + \frac{7}{4}\zeta(3)\log^2(2) + \frac{1}{18}\pi^2\log^3(2) - \frac{1}{8}\pi^2\zeta(3)$$

Dozens of general and specific results have now been established.

Authors: Jonathan Borwein, David Borwein, Roland Girgensohn and DHB

Apery-Like Identities

The following were recently found using extensive integer relation searches:

$$\begin{aligned}
\zeta(5) &= 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2}, \\
\zeta(7) &= \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} \\
\zeta(9) &= \frac{9}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^9\binom{2k}{k}} - \frac{5}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2} + 5\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} \\
&\quad + \frac{45}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^6} - \frac{25}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{j=1}^{k-1}\frac{1}{j^2},
\end{aligned}$$

$$\sum_{n=0}^{\infty}\zeta(4n+3)x^{4n} = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}(1-x^4/k^4)}\prod_{m=1}^{k-1}\left(\frac{1+4x^4/m^4}{1-x^4/m^4}\right)$$

Authors: Jonathan Borwein and David Bradley

New Apery-Like Identities (Nov 2005)

Following an even more extensive "bootstrapping" experimental approach, similar results have now been found for found for zeta(2n):

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^2}$$

$$\zeta(4) = 3\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^4} - 9\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^2}$$

$$\zeta(6) = 3\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^6} - 9\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^4} - \frac{45}{2}\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-4}}{\binom{2k}{k}k^2} + \frac{27}{2}\sum_{k=1}^{\infty}\sum_{j=1}^{k-1}\frac{\sum_{i=1}^{k-1} i^{-2}}{j^2\binom{2k}{k}k^2}$$

$$\sum_{n=0}^{\infty}\zeta(2n+2)x^{2n} = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}\left(1-x^2/k^2\right)}\prod_{m=1}^{k-1}\left(\frac{1-4x^2/m^2}{1-x^2/m^2}\right)$$

Authors: Jonathan Borwein, David Bradley and DHB

Ramanujan-Like Identities

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (13 + 180n + 820n^2) \left(\frac{1}{32}\right)^{2n}$$

$$\frac{32}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (1 + 8n + 20n^2) \left(\frac{1}{2}\right)^{2n}$$

$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r(n)^7 (1 + 14n + 76n^2 + 168n^3) \left(\frac{1}{32}\right)^{2n}$$

where

$$r(n) = \frac{(1/2)_n}{n!} = \frac{1/2 \cdot 3/2 \cdot \cdots \cdot (2n-1)/2}{n!} = \frac{\Gamma(n+1/2)}{\sqrt{\pi}\,\Gamma(n+1)}$$

Numerous additional results could be listed.

Authors: Jesus Guillera and B. Gourevitch

A Connection Between BBP Formulas and Normality

Consider the “chaotic” sequence defined by $x_0 = 0$, and

$$x_n = \left\{2x_{n-1} + \frac{1}{n}\right\}$$

where { } denotes fractional part as before.

Result: log(2) is 2-normal if and only if this sequence is equidistributed in the unit interval.

In a similar vein, consider the sequence $x_0 = 0$, and

$$x_n = \left\{16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21}\right\}$$

Result: π is 16-normal if and only if this sequence is equidistributed in the unit interval.

Authors: Richard Crandall and DHB

A Class of Provably Normal Constants

We have also shown that an infinite class of mathematical constants is normal, including

$$\alpha_{2,3} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}}$$
$$= 0.041883680831502985071252898624571682426096\ldots_{10}$$
$$= 0.0\mathtt{AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0}\ldots_{16}$$

$\alpha_{2,3}$ was proven 2-normal by Stoneham in 1971, but we have extended this to the case where (2,3) are any pair (p,q) of relatively prime integers. We also extended to an uncountably infinite class, as follows [here r_k is the k-th bit of r in (0,1)]:

$$\alpha_{2,3}(r) = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k + r_k}}$$

This result has led to a practical and effective pseudo-random number generator based on the binary digits of $\alpha_{2,3}$.

Authors: Richard Crandall and DHB

The "Hot Spot" Lemma for Proving Normality (2005)

Recently we were able to prove normality for these alpha constants very simply, by means of a new result that we call the "hot spot" lemma, proven using ergodic theory:

Hot Spot Lemma: Let {} denote fractional part. Then x is b-normal if and only if there is no y in [0,1) such that

$$\liminf_{m\to\infty} \limsup_{n\to\infty} \frac{\#_{0\le j<n}(|\{b^j x\} - y| < b^{-m})}{2nb^{-m}} = \infty$$

Paraphrase: x is b-normal if and only if it has no base-b hot spots.

Sample Corollary: If, for each m and n, no m-long string of digits appears in the first n digits of the base-2 expansion of x more often than 1,000 n 2^{-m} times, then x is 2-normal.

Authors: Michal Misiurewicz and DHB

Experimental Math as Applied Mathematics

- The ultimate objective is to advance the applied discipline:
  - Here the “applied discipline” is pure mathematics!
- Advanced numerical algorithms and computational techniques:
  - PSLQ, high-precision arithmetic, symbolic computing, FFTs, numerical analysis, evaluation of integrals and series, etc.
- State-of-the-art calculations require highly parallel computers:
  - High-precision arithmetic greatly magnifies run times.
  - 1000+ CPUs have been used in several calculations.
- A pragmatic attitude prevails: “If it works, use it.”
  - We do not know ahead of time what terms to use in an integer relation search – guessing which terms to try is still a black art.
  - Whereas the standard PSLQ algorithm is guaranteed to find relations, no proof is known for multi-pair PSLQ.
  - We do not fully understand tanh-sinh quadrature, especially in 2-D.

Computational Methods Used in Experimental Math

- High-precision computation.
- PSLQ.
- Symbolic computing tools.
- Function evaluations: sin, exp, log, erf, gamma, zeta, polylog.
- Fast Fourier transforms (FFTs).
- Dense and sparse linear algebra.
- Evaluation of definite integrals.
- Evaluation of infinite series sums.
- Error bounds on computed results.
- Highly parallel computing.
- Computer graphics.

Except for high-precision arithmetic and PSLQ, these are all staples of applied mathematics and numerical analysis.

Experimental math is a driver for advanced numerical analysis research.

FFTs in Experimental Math

FFTs are used in high-precision arithmetic software packages (including ARPREC) to accelerate multiplication:

- Multiplication, except for releasing carries, is merely a linear convolution, which can be efficiently computed using FFTs.
- Division can exploit FFT-based multiplication via Newton iterations.

FFTs may also be used to accelerate polynomial multiplication and division. Example: We can calculate a large set of even zeta values (and also even Bernoulli numbers) as follows:

$$\frac{-2}{\pi x}\sum_{k=0}^{\infty}\zeta(2k)(-1)^k x^{2k} = \coth(\pi x) = \cosh(\pi x)/\sinh(\pi x)$$

$$= \frac{1}{\pi x}\cdot\frac{1+(\pi x)^2/2!+(\pi x)^4/4!+(\pi x)^6/6!+\cdots}{1+(\pi x)^2/3!+(\pi x)^4/5!+(\pi x)^6/7!+\cdots}.$$

The polynomial division here can be performed using Newton iterations, where polynomial multiplications are performed using FFTs.

Authors: Jonathan Borwein, Richard Crandall and DHB

LBNL's High-Precision Software (ARPREC and QD)

- Low-level routines written in C++.
- C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) available.
- Special routines for extra-high precision (>1000 dig).
- Includes common math functions: sqrt, cos, exp, etc.
- PSLQ, root finding, numerical integration.
- An interactive "Experimental Mathematician's Toolkit" employing this software is also available.

Available at: **`http://www.experimentalmath.info`**

This software is now being used by physicists, climate modelers, chemists and engineers, in addition to mathematicians.

Authors: Xiaoye Li, Yozo Hida, Brandon Thompson and DHB

The Euler-Maclaurin Formula of Numerical Analysis

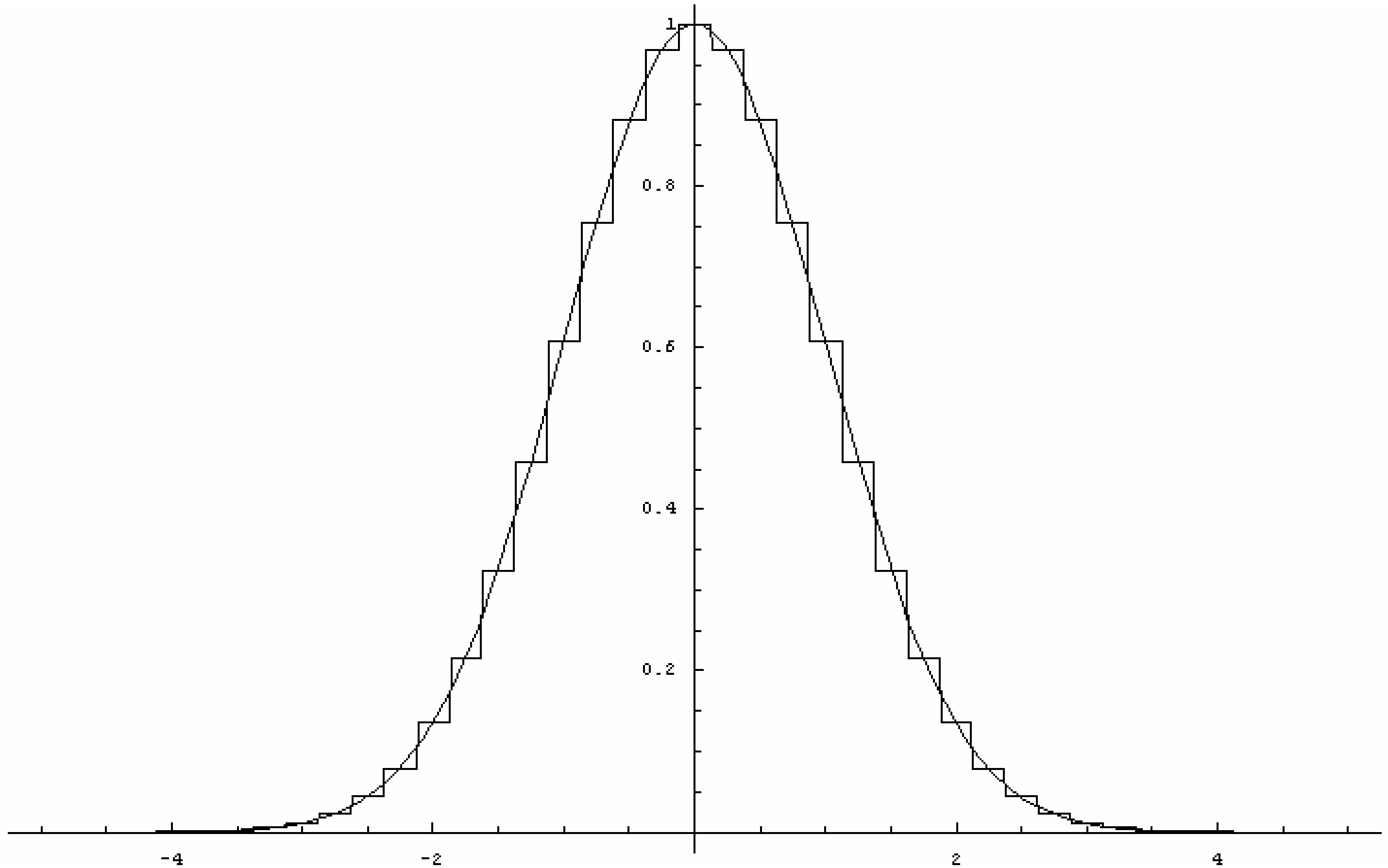
$$
\begin{aligned}
\int_a^b f(x)\,dx &= h \sum_{j=0}^{n} f(x_j) - \frac{h}{2}\left(f(a) + f(b)\right) \\
&\quad - \sum_{i=1}^{m} \frac{h^{2i} B_{2i}}{(2i)!} \left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right) - E(h) \\
|E(h)| &\le 2(b-a)[h/(2\pi)]^{2m+2} \max_{a \le x \le b} |D^{2m+2} f(x)|
\end{aligned}
$$

[Here h = (b - a)/n and x_j = a + j h. D^m f(x) means m-th derivative of f.]

Note when f(t) and all of its derivatives are zero at a and b, the error E(h) of a simple block-function approximation to the integral goes to zero more rapidly than any power of h.

Reference: Kendall Atkinson, *An Introduction to Numerical Analysis*

Block-Function Approximation to the Integral of a Bell-Shaped Function



High-Precision Integration and the Euler-Maclaurin Formula

Given f(x) defined on (-1,1), employ a function g(t) such that g(t) goes from -1 to 1 over the real line, with g'(t) going to zero for large |t|. Then x = g(t) yields

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;\approx\; h\sum_{-N}^{N} w_j f(x_j)$$

Here $x_j = g(hj)$ and $w_j = g'(hj)$. If g'(t) goes to zero rapidly enough for large t, then even if f(x) has a vertical derivative or blow-up singularity at an endpoint, the product f(g(t)) g'(t) usually is a nice bell-shaped function for which the E-M formula applies.

Such schemes often achieve quadratic convergence – reducing h by half produces twice as many correct digits.

Authors: Xiaoye Li, Karthik Jeyabalan and DHB

Four Suitable ‘g’ Functions

$$
\begin{aligned}
g(t) &= \operatorname{erf}(t) & g'(t) &= \frac{2}{\sqrt{\pi}} e^{-t^2} \\
g(t) &= \tanh t & g'(t) &= \frac{1}{\cosh^2 t} \\
g(t) &= \tanh(\sinh t) & g'(t) &= \frac{\sinh t}{\cosh^2(\sinh t)} \\
g(t) &= \tanh(\pi/2 \cdot \sinh t) & g'(t) &= \frac{\pi/2 \cdot \sinh t}{\cosh^2(\pi/2 \cdot \sinh t)}
\end{aligned}
$$

Tanh-sinh quadrature uses one of the last two formulas.

Error Estimation in Tanh-Sinh Quadrature (Dec 2005)

Let F(t) be the desired integrand function on [a,b]. Define f(t) = F(g(t)) g'(t), where g(t) = tanh (sinh t) (or one of the other g functions above). Then a very accurate estimate of the error of the quadrature result is:

$$E_2(h,m) \;=\; h(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m} f(jh)$$

First order (m = 1) estimates are remarkably accurate. Higher-order estimates (m > 1) can be used to obtain rigorous “certificates” on the accuracy of a tanh-sinh quadrature result.

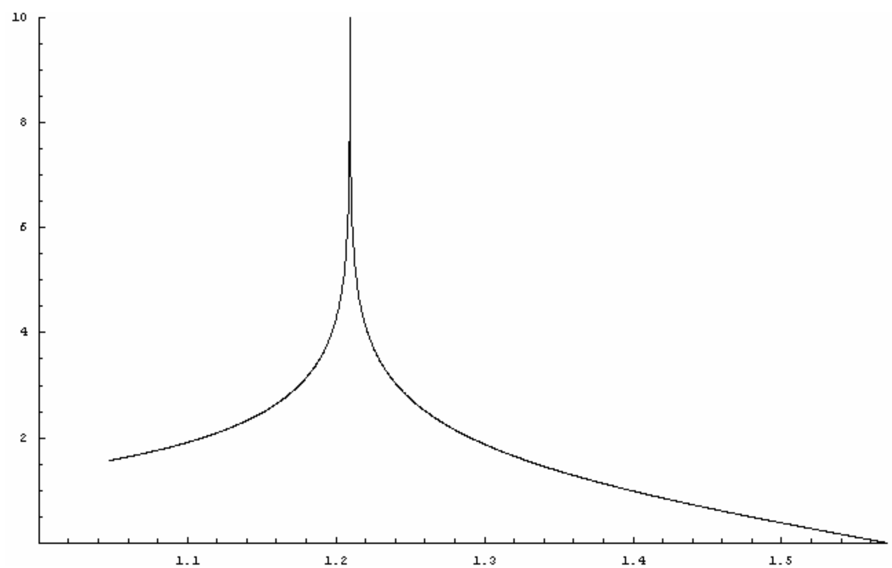
This formula was originally discovered due to a “bug” in our computer program.

Authors: Jonathan Borwein and DHB

Application of High-Precision Tanh-Sinh Quadrature

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt$$
$$\stackrel{?}{=} \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This arises from analysis of volumes of ideal tetrahedra in hyperbolic space. This "identity" has now been verified numerically to 20,000 digits, but no proof is known. Note that the integrand function has a nasty singularity.



Authors: Jonathan Borwein, David Broadhurst and DHB

Ising Theory Integrals
(Apr 2006)

The following integrals arise in Ising theory of mathematical physics:

$$C_n = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

Richard Crandall showed that this can be transformed to a 1-D integral:

$$C_n = \frac{2^n}{n!} \int_0^\infty t K_0^n(t) \; dt$$

where K_0 is a modified Bessel function. We then computed 400-digit numerical values, from which these results were found (and proven):

$$\begin{aligned} C_3 &= \mathrm{L}_{-3}(2) = \sum_{n \ge 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right) \\ C_4 &= 14\zeta(3) \\ \lim_{n \to \infty} C_n &= 2e^{-2\gamma} \end{aligned}$$

Authors: Jonathan Borwein, Richard Crandall and DHB

Box Integrals (Apr 2006)

Spurred by a question posed in January 2006 by Luis Goddyn of SFU, we examined some related integrals of the form:

$$B_n(s) = \int_0^1 \cdots \int_0^1 \left(r_1^2 + \ldots + r_n^2\right)^{s/2} dr_1 \cdots dr_n$$

The following evaluations are now known:

$$B_1(1) = \frac{1}{2}$$

$$B_2(1) = \frac{\sqrt{2}}{3} + \frac{1}{3}\log\left(\sqrt{2}+1\right)$$

$$B_3(1) = \frac{\sqrt{3}}{4} + \frac{1}{2}\log\left(2+\sqrt{3}\right) - \frac{\pi}{24}$$

$$B_4(1) = \frac{2}{5} + \frac{7}{20}\pi\sqrt{2} - \frac{1}{20}\pi\log\left(1+\sqrt{2}\right) + \log(3) - \frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right) + \frac{1}{10}\mathcal{K}_0$$

where

$$\mathcal{K}_0 = \int_0^1 \frac{\log(1+\sqrt{3+y^2}) - \log(-1+\sqrt{3+y^2})}{1+y^2}\,dy$$

Authors: Jonathan Borwein, Richard Crandall and DHB

Some Supercomputer-Class Experimental Math Computations

Identification of B_4, the fourth bifurcation point of the logistic iteration.

- Integer relation of size 121; 10,000 digit arithmetic.

Identification of Euler-zeta sums.

- Hundreds of integer relation problems, each of size 145 and requiring 5,000 digit arithmetic.
- Run on IBM SP parallel system – many hours run time.

Finding relation involving root of Lehmer's polynomial.

- Integer relation of size 125; 50,000 digit arithmetic.
- Required 16 hours on 64 CPUs of the Seaborg system at LBNL.

Numerical verification of a mathematical physics integral identity.

- 1-D quadrature calculation; 20,000-digit arithmetic.
- Required 45 min on 1024 CPUs of the Apple system at Virginia Tech.

Numerical evaluation of an Ising theory integral.

- 3-D quadrature of a very complicated function; 500-digit arithmetic.
- Required 18.2 hours on 256 CPUs of the Bassi system at LBNL.

Authors: David Broadhurst, Jonathan Borwein, Richard Crandall, Roland Girgensohn and DHB

One of the Ising Integrals (Evaluated to 250-Digit Precision)

$$
\begin{aligned}
E_5 = \int_0^1\int_0^1\int_0^1 & [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z((y^2+1)z^2+4(y+ \\
& 1)z+5)x^5 + y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4 + y(z(z^2+4z+5)y^2+4(z^2+1)y+5z+4)x^3 + ((-3z^2-4z+1)y^2-4zy+1)x^2 \\
& -(y(5z+4)+4)x-1)]/[(x-1)^3(xy-1)^3(xyz-1)^3] + [3(y-1)^2y^4(z-1)^2z^2(yz-1)^2x^6 + 2y^3z(3(z-1)^2z^3y^5+z^2(5z^3+3z^2+3z+5)y^4+(z-1)^2z \\
& (5z^2+16z+5)y^3 + (3z^5+3z^4-22z^3-22z^2+3z+3)y^2 + 3(-2z^4+z^3+2z^2+z-2)y+3z^3+5z^2+5z+3)x^5 + y^2(7(z-1)^2z^4y^6-2z^3(z^3+15z^2 \\
& +15z+1)y^5 + 2z^2(-21z^4+6z^3+14z^2+6z-21)y^4 - 2z(z^5-6z^4-27z^3-27z^2-6z+1)y^3 + (7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2 - 2(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)y+7z^4-2z^3-42z^2-2z+7)x^4 - 2y(z^3(z^3-9z^2-9z+1)y^6+z^2(7z^4-14z^3-18z^2-14z+7)y^5+z(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)y^4 + (z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3 - 3(3z^5+6z^4-z^3-z^2+6z+3)y^2 - (9z^4+14z^3-14z^2+14z+9)y+z^3+7z^2+7z \\
& +1)x^3 + (z^2(11z^4+6z^3-66z^2+6z+11)y^6+2z(5z^5+13z^4-2z^3-2z^2+13z+5)y^5 + (11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4 + (6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)y^3 - 2(33z^4+2z^3-22z^2+2z+33)y^2 + (6z^3+26z^2+26z+6)y+11z^2+10z+11)x^2 - 2(z^2(5z^3+3z^2+3z+5)y^5+z(22z^4 \\
& +5z^3-22z^2+5z+22)y^4 + (5z^5+5z^4-26z^3-26z^2+5z+5)y^3 + (3z^4-22z^3-26z^2-22z+3)y^2 + (3z^3+5z^2+5z+3)y+5z^2+22z+5)x+15z^2+2z \\
& +2y(z-1)^2(z+1)+2y^3(z-1)^2z(z+1)+y^4z^2(15z^2+2z+15)+y^2(15z^4-2z^3-90z^2-2z+15)+15]/[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2] - [4(x+1)(y+1)(yz+1)(-z^2y^4+4z(z+1)y^3+(z^2+1)y^2-4(z+1)y+4x(y^2-1)(y^2z^2-1)+x^2(z^2y^4-4z(z+1)y^3-(z^2+1)y^2 \\
& +4(z+1)y+1)-1)\log(x+1)]/[(x-1)^3x(y-1)^3(yz-1)^3] - [4(y+1)(xy+1)(z+1)(x^2(z^2-4z-1)y^4+4x(x+1)(z^2-1)y^3-(x^2+1)(z^2-4z-1) \\
& y^2-4(x+1)(z^2-1)y+z^2-4z-1)\log(xy+1)]/[x(y-1)^3y(xy-1)^3(z-1)^3] - [4(z+1)(yz+1)(x^3y^5z^7+x^2y^4(4x(y+1)+5)z^6-xy^3((y^2+ \\
& 1)x^2-4(y+1)x-3)z^5-y^2(4y(y+1)x^3+5(y^2+1)x^2+4(y+1)x+1)z^4+y(y^2x^3-4y(y+1)x^2-3(y^2+1)x-4(y+1))z^3+(5x^2y^2+y^2+4x(y+1) \\
& y+1)z^2+((3x+4)y+4)z-1)\log(xyz+1)]/[xy(z-1)^3z(yz-1)^3(xyz-1)^3])]/[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2] \\
& dx\,du\,dz
\end{aligned}
$$

Pure or Applied Mathematics?

Experimental math can be described as applied mathematics, where the principal applied discipline is pure mathematics – it is both pure and applied mathematics.

Other applied aspects of experimental math:

- Several of the recent results are in mathematical physics.
- The BBP formula for pi is now used in the G95 compiler.
- High-precision software is now being used in physics, chemistry, climate modeling and engineering.
- The normal number result has led to an efficient pseudo-random number generator, used for instance in the new DOD-DOE high-performance computing benchmarks.

The Appeal of Experimental Math

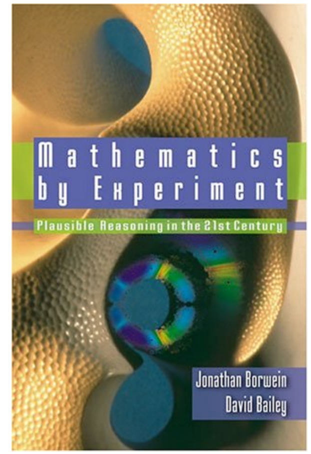
- Experimental math is accessible.
  - Much is readily understandable to persons with only modest mathematical backgrounds.
- Experimental math is multidisciplinary.
  - Mathematicians, numerical analysts, computer scientists, and physicists have all made significant contributions.
- Experimental math excites the younger, computer-savvy generation.
  - Students with good programming skills can do real research.
- Experimental math is an excellent tool for student learning.
  - With a few experiments, students can “see” what’s happening.
  - Computer graphics and plots are particularly useful.
  - Student versions of *Mathematica* and *Maple* are now available at very reasonable prices.

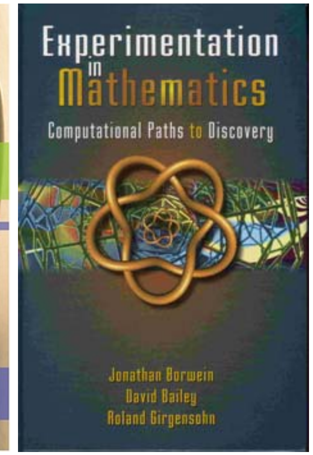
Books on Experimental Mathematics

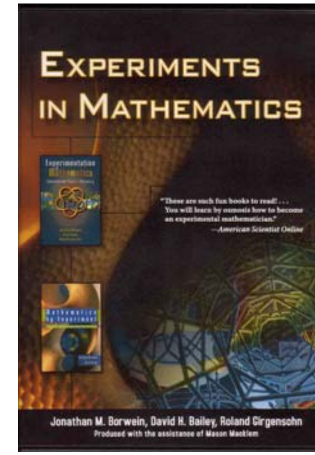
Vol. 1: *Mathematics by Experiment: Plausible Reasoning in the 21st Century*

Vol. 2: *Experiments in Mathematics: Computational Paths to Discovery*

Authors: Jonathan Borwein, DHB and (for vol. 2) Roland Girgensohn.







New: Both books are now available on CD-ROM in a hyperlinked, searchable PDF format. Also, a FREE condensed version is available at: **`http://www.experimentalmath.info`**

Coming soon: *Experimental Mathematics in Action*.
Authors: David Bailey, Jon Borwein, Neil Calder, Roland Girgensohn, Russell Luke and Victor Moll.